wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2024 – 03:02 PM EDT

PDB ID	:	3RIK
Title	:	The acid beta-glucosidase active site exhibits plasticity in binding 3,4,5,6-tetra hydroxyazepane-based inhibitors: implications for pharmacological chaperone design for gaucher disease
Authors	:	Orwig, S.D.; Lieberman, R.L.
Deposited on	:	2011-04-13
Resolution	:	2.48 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

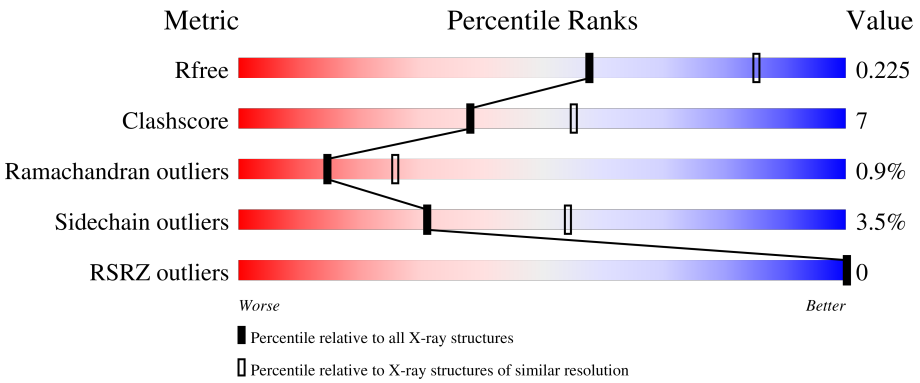
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	82% 15% • •
1	B	497	85% 13% • •
1	C	497	86% 12% • •
1	D	497	84% 15% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16878 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

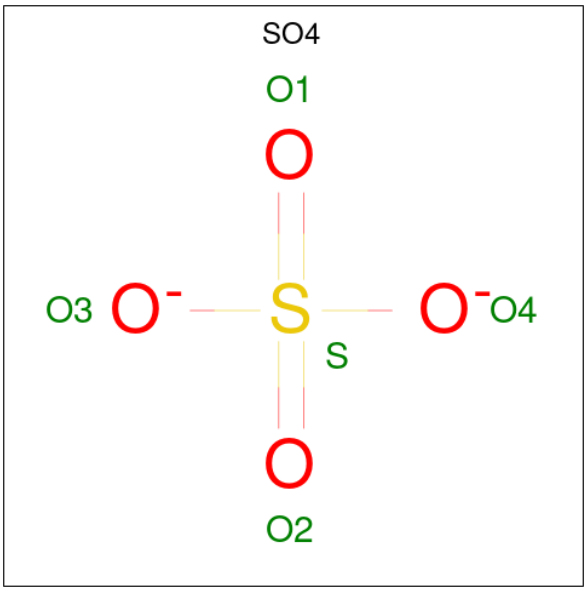
- Molecule 1 is a protein called Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3929	2532	671	710	16	0	0	0
1	B	497	3929	2532	671	710	16	0	0	0
1	C	497	3929	2532	671	710	16	0	0	0
1	D	497	3929	2532	671	710	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	variant	UNP P04062
B	495	HIS	ARG	variant	UNP P04062
C	495	HIS	ARG	variant	UNP P04062
D	495	HIS	ARG	variant	UNP P04062

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



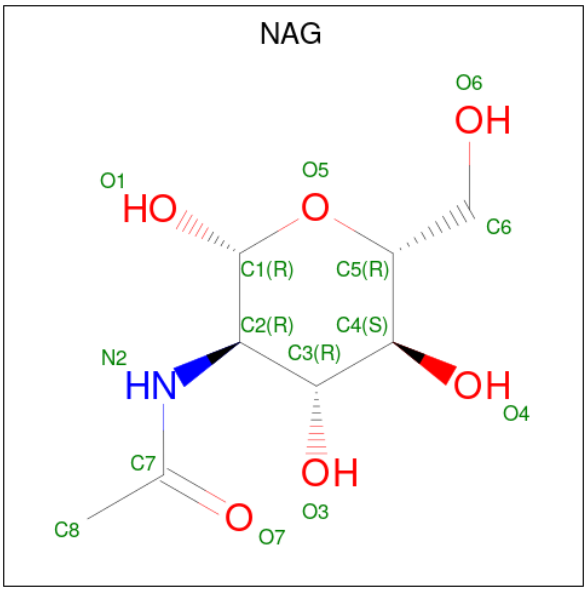
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0

Continued on next page...

Continued from previous page...

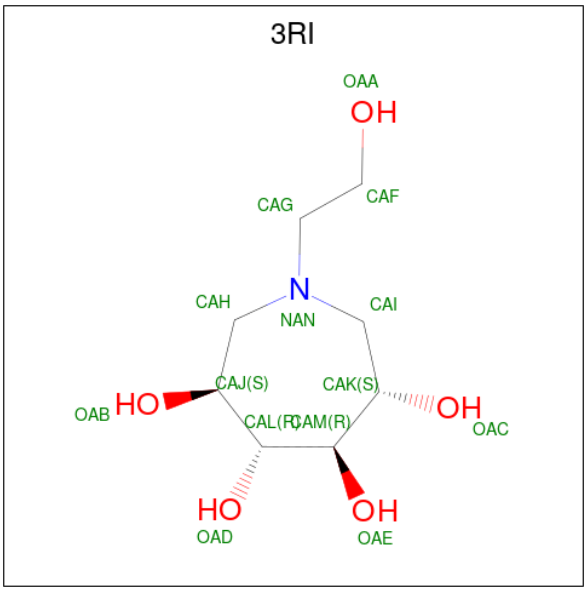
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0
			Total	C	N	O		
3	C	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0

- Molecule 4 is (3S,4R,5R,6S)-1-(2-hydroxyethyl)azepane-3,4,5,6-tetrol (three-letter code: 3RI) (formula: $C_8H_{17}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	D	1	14	8	1	5	0	0

- Molecule 5 is water.

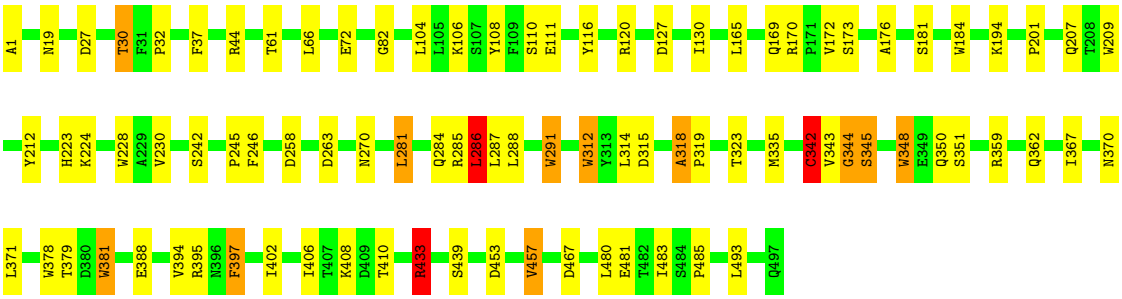
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	232	232	232	0	0
			Total	O		
5	B	233	233	233	0	0
			Total	O		
5	C	228	228	228	0	0
			Total	O		
5	D	215	215	215	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

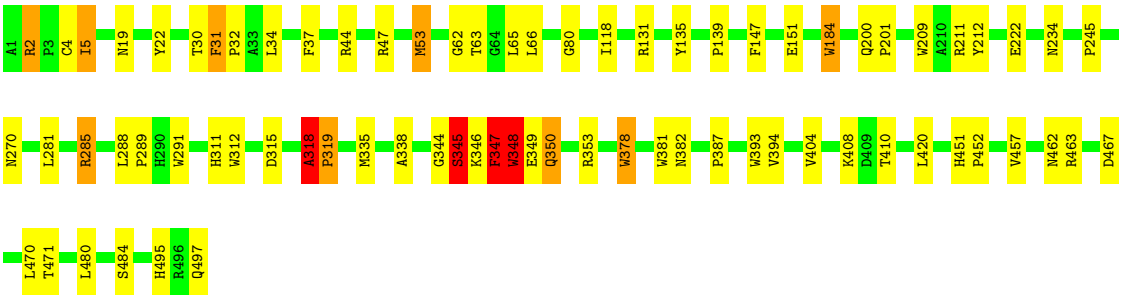
- Molecule 1: Glucosylceramidase

Chain A:



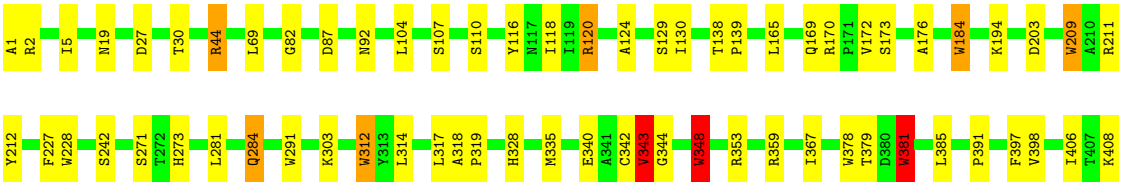
- Molecule 1: Glucosylceramidase

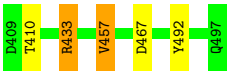
Chain B:



- Molecule 1: Glucosylceramidase

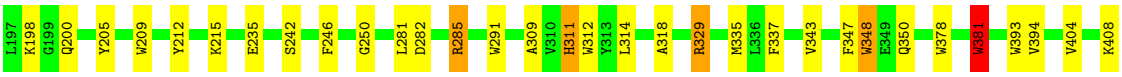
Chain C:





- Molecule 1: Glucosylceramidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.98Å 91.55Å 152.21Å 90.00° 110.70° 90.00°	Depositor
Resolution (Å)	46.50 – 2.48 46.50 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.3 (46.50-2.48) 94.3 (46.50-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.225 0.162 , 0.225	Depositor DCC
R_{free} test set	4628 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 17.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16878	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3RI, SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.87	5/4050 (0.1%)	0.88	4/5523 (0.1%)
1	B	0.88	6/4050 (0.1%)	0.88	5/5523 (0.1%)
1	C	0.89	8/4050 (0.2%)	0.87	4/5523 (0.1%)
1	D	0.90	7/4050 (0.2%)	0.85	1/5523 (0.0%)
All	All	0.89	26/16200 (0.2%)	0.87	14/22092 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	TRP	CD2-CE2	8.14	1.51	1.41
1	D	348	TRP	CD2-CE2	7.96	1.50	1.41
1	D	393	TRP	CD2-CE2	7.50	1.50	1.41
1	B	184	TRP	CD2-CE2	7.28	1.50	1.41
1	B	291	TRP	CD2-CE2	7.04	1.49	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	433	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	A	433	ARG	NE-CZ-NH2	-7.53	116.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	285	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	318	ALA	C-N-CD	-6.98	105.24	120.60
1	B	5	ILE	CG1-CB-CG2	-6.74	96.56	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	CYS	Peptide
1	B	347	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3929	0	3843	66	0
1	B	3929	0	3844	58	0
1	C	3929	0	3844	41	0
1	D	3929	0	3844	50	0
2	A	50	0	0	0	0
2	B	40	0	0	0	0
2	C	45	0	0	3	0
2	D	35	0	0	1	0
3	A	14	0	13	0	0
3	B	14	0	13	3	0
3	C	14	0	13	3	0
3	D	14	0	13	2	0
4	B	14	0	17	0	0
4	D	14	0	17	1	0
5	A	232	0	0	5	0
5	B	233	0	0	8	0
5	C	228	0	0	4	0
5	D	215	0	0	6	0
All	All	16878	0	15461	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 212 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ASN:HD21	3:D:509:NAG:C1	1.10	1.58
1:B:19:ASN:HD21	3:B:510:NAG:C1	1.02	1.55
1:C:19:ASN:HD21	3:C:510:NAG:C1	1.28	1.47
1:D:329:ARG:HH11	1:D:329:ARG:HG2	1.06	1.05
1:A:344:GLY:HA2	1:A:345:SER:HB3	1.38	1.04

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/497 (100%)	467 (94%)	23 (5%)	5 (1%)	13	23
1	B	495/497 (100%)	465 (94%)	23 (5%)	7 (1%)	9	16
1	C	495/497 (100%)	468 (94%)	23 (5%)	4 (1%)	16	29
1	D	495/497 (100%)	472 (95%)	21 (4%)	2 (0%)	30	47
All	All	1980/1988 (100%)	1872 (94%)	90 (4%)	18 (1%)	14	26

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	ALA
1	A	345	SER
1	B	318	ALA
1	B	347	PHE
1	C	343	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/424 (100%)	412 (97%)	12 (3%)	38	63
1	B	424/424 (100%)	408 (96%)	16 (4%)	28	50
1	C	424/424 (100%)	409 (96%)	15 (4%)	31	54
1	D	424/424 (100%)	408 (96%)	16 (4%)	28	50
All	All	1696/1696 (100%)	1637 (96%)	59 (4%)	31	54

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	ARG
1	D	441	LYS
1	C	335	MET
1	D	394	VAL
1	D	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	60	HIS
1	C	396	ASN
1	D	495	HIS
1	C	328	HIS
1	C	497	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

40 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	506	-	4,4,4	0.50	0	6,6,6	0.42	0
2	SO4	A	501	-	4,4,4	0.50	0	6,6,6	0.85	0
2	SO4	A	505	-	4,4,4	0.60	0	6,6,6	0.36	0
2	SO4	B	502	-	4,4,4	0.29	0	6,6,6	0.83	0
2	SO4	B	504	-	4,4,4	0.53	0	6,6,6	0.53	0
2	SO4	A	506	-	4,4,4	0.38	0	6,6,6	0.63	0
3	NAG	A	511	1	14,14,15	0.45	0	17,19,21	0.79	0
2	SO4	C	505	-	4,4,4	0.35	0	6,6,6	0.51	0
3	NAG	C	510	1	14,14,15	1.60	2 (14%)	17,19,21	2.29	5 (29%)
2	SO4	B	503	-	4,4,4	0.45	0	6,6,6	0.52	0
2	SO4	D	505	-	4,4,4	0.38	0	6,6,6	0.21	0
2	SO4	A	510	-	4,4,4	0.55	0	6,6,6	0.34	0
2	SO4	B	509	-	4,4,4	0.51	0	6,6,6	0.34	0
2	SO4	D	508	-	4,4,4	0.54	0	6,6,6	0.30	0
3	NAG	D	509	1	14,14,15	2.03	4 (28%)	17,19,21	2.54	7 (41%)
2	SO4	A	504	-	4,4,4	0.56	0	6,6,6	0.48	0
2	SO4	A	503	-	4,4,4	0.54	0	6,6,6	0.51	0
2	SO4	D	502	-	4,4,4	0.55	0	6,6,6	0.48	0
2	SO4	A	509	-	4,4,4	0.52	0	6,6,6	0.43	0
2	SO4	D	506	-	4,4,4	0.57	0	6,6,6	0.57	0
2	SO4	A	508	-	4,4,4	0.50	0	6,6,6	0.82	0
2	SO4	C	501	-	4,4,4	0.64	0	6,6,6	0.70	0
2	SO4	C	502	-	4,4,4	0.65	0	6,6,6	0.74	0
2	SO4	C	504	-	4,4,4	0.51	0	6,6,6	0.56	0
4	3RI	B	501	-	12,14,14	1.05	0	10,19,19	1.01	1 (10%)
2	SO4	C	506	-	4,4,4	0.48	0	6,6,6	0.31	0
2	SO4	B	507	-	4,4,4	0.53	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	504	-	4,4,4	0.55	0	6,6,6	0.84	0
2	SO4	D	503	-	4,4,4	0.55	0	6,6,6	0.63	0
2	SO4	D	507	-	4,4,4	0.51	0	6,6,6	0.26	0
2	SO4	C	503	-	4,4,4	0.44	0	6,6,6	0.54	0
2	SO4	C	509	-	4,4,4	0.49	0	6,6,6	0.27	0
2	SO4	A	502	-	4,4,4	0.68	0	6,6,6	0.70	0
4	3RI	D	501	-	12,14,14	0.77	0	10,19,19	0.95	0
2	SO4	B	505	-	4,4,4	0.46	0	6,6,6	0.37	0
2	SO4	C	507	-	4,4,4	0.48	0	6,6,6	0.53	0
3	NAG	B	510	1	14,14,15	1.96	5 (35%)	17,19,21	2.08	7 (41%)
2	SO4	B	508	-	4,4,4	0.51	0	6,6,6	0.11	0
2	SO4	A	507	-	4,4,4	0.53	0	6,6,6	0.24	0
2	SO4	C	508	-	4,4,4	0.59	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	510	1	-	1/6/23/26	0/1/1/1
4	3RI	D	501	-	-	1/3/23/23	0/1/1/1
4	3RI	B	501	-	-	1/3/23/23	0/1/1/1
3	NAG	B	510	1	-	2/6/23/26	0/1/1/1
3	NAG	D	509	1	-	1/6/23/26	0/1/1/1
3	NAG	A	511	1	-	0/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	509	NAG	O4-C4	4.74	1.54	1.43
3	B	510	NAG	O4-C4	4.02	1.52	1.43
3	D	509	NAG	O5-C5	3.99	1.51	1.43
3	C	510	NAG	O4-C4	3.51	1.51	1.43
3	C	510	NAG	O5-C5	3.43	1.50	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	509	NAG	C1-O5-C5	6.57	120.99	112.19
3	B	510	NAG	O5-C5-C6	-5.25	97.45	107.66
3	C	510	NAG	C1-O5-C5	4.54	118.27	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	510	NAG	C6-C5-C4	-4.35	102.34	113.02
3	D	509	NAG	C6-C5-C4	-4.16	102.80	113.02

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	3RI	OAA-CAF-CAG-NAN
4	D	501	3RI	OAA-CAF-CAG-NAN
3	B	510	NAG	C4-C5-C6-O6
3	D	509	NAG	C4-C5-C6-O6
3	C	510	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	505	SO4	1	0
3	C	510	NAG	3	0
3	D	509	NAG	2	0
2	C	501	SO4	1	0
2	C	506	SO4	1	0
2	D	503	SO4	1	0
4	D	501	3RI	1	0
3	B	510	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	497/497 (100%)	-1.89	0	100	100	15, 23, 45, 83	0
1	B	497/497 (100%)	-1.86	0	100	100	14, 25, 49, 93	0
1	C	497/497 (100%)	-1.89	0	100	100	14, 24, 46, 71	0
1	D	497/497 (100%)	-1.86	0	100	100	15, 25, 52, 93	0
All	All	1988/1988 (100%)	-1.87	0	100	100	14, 24, 47, 93	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	510	5/5	0.97	0.05	78,88,96,106	0
2	SO4	D	508	5/5	0.97	0.05	75,79,87,92	0
2	SO4	C	506	5/5	0.98	0.05	78,82,86,88	0
2	SO4	C	507	5/5	0.98	0.06	69,79,87,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	508	5/5	0.98	0.04	83,89,92,96	0
2	SO4	C	509	5/5	0.98	0.07	66,70,74,82	0
2	SO4	B	509	5/5	0.98	0.04	81,82,95,108	0
3	NAG	A	511	14/15	0.98	0.04	37,44,51,58	0
3	NAG	C	510	14/15	0.98	0.04	41,44,50,55	0
2	SO4	B	506	5/5	0.99	0.05	82,83,86,88	0
2	SO4	B	507	5/5	0.99	0.03	83,84,92,102	0
2	SO4	B	508	5/5	0.99	0.04	77,95,96,97	0
2	SO4	A	505	5/5	0.99	0.04	54,59,62,63	0
2	SO4	C	503	5/5	0.99	0.04	53,55,58,61	0
2	SO4	C	504	5/5	0.99	0.06	51,51,55,58	0
2	SO4	C	505	5/5	0.99	0.07	60,62,67,74	0
2	SO4	A	506	5/5	0.99	0.07	53,61,72,76	0
2	SO4	A	507	5/5	0.99	0.06	64,66,72,83	0
2	SO4	A	508	5/5	0.99	0.06	65,66,75,80	0
2	SO4	A	504	5/5	0.99	0.03	50,51,54,61	0
2	SO4	D	503	5/5	0.99	0.03	46,47,51,52	0
2	SO4	D	504	5/5	0.99	0.03	45,48,54,54	0
2	SO4	D	506	5/5	0.99	0.04	66,69,69,76	0
2	SO4	D	507	5/5	0.99	0.05	72,73,79,94	0
2	SO4	B	503	5/5	0.99	0.03	50,51,51,55	0
2	SO4	B	504	5/5	0.99	0.03	46,48,54,54	0
3	NAG	B	510	14/15	0.99	0.04	32,38,41,48	0
2	SO4	B	505	5/5	0.99	0.04	59,65,68,72	0
3	NAG	D	509	14/15	0.99	0.04	36,41,46,48	0
2	SO4	A	503	5/5	1.00	0.06	51,54,55,59	0
2	SO4	D	505	5/5	1.00	0.02	61,63,68,68	0
2	SO4	B	502	5/5	1.00	0.02	30,30,34,35	0
2	SO4	A	501	5/5	1.00	0.02	30,31,33,34	0
2	SO4	A	502	5/5	1.00	0.01	42,42,49,50	0
2	SO4	C	501	5/5	1.00	0.02	22,22,23,23	0
2	SO4	C	502	5/5	1.00	0.02	42,43,50,54	0
2	SO4	D	502	5/5	1.00	0.01	23,26,28,29	0
2	SO4	A	509	5/5	1.00	0.04	50,60,61,65	0
4	3RI	B	501	14/14	1.00	0.02	25,32,43,44	0
4	3RI	D	501	14/14	1.00	0.02	28,34,43,44	0

6.5 Other polymers (i)

There are no such residues in this entry.